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Zondervan, Edwin; Roffel, Brian

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Dynamic optimization of chemical cleaning in dead-end ultra filtration

Edwin Zondervan*, Brian Roffel

*Department of Chemical Engineering, Research Institute for Management and Technology, University of Groningen, Nijenborgh 4,
9747 AG Groningen, The Netherlands*

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Abstract

In this paper a control strategy is formulated that minimizes the costs for a single chemical cleaning of a dead-end ultra filtration membrane. From the process model, the performance index and the constraints it can be derived that dynamic optimization will lead to a ‘maximum effort control problem’, in which the controls (cleaning flow and cleaning agent concentration) are either zero or maximum. The change from maximum to zero is called the switching point. This switching point depends on the overall cleaning time and the requested cleaning effectiveness. From the calculated optimal control strategy it follows that cleaning time can be significantly reduced, compared to conventional cleaning.

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Keywords: Ultra filtration; Chemical cleaning; Modeling; Dynamic optimization

1. Introduction

Ultra filtration (UF) is a promising technology in the field of surface water purification. UF membranes are easy to scale-up and became economically attractive in the last 15 years. However, membrane performance is often limited by fouling. Fouling components present in surface water attach to the membrane and need to be frequently removed by means of backwashes and in the long term the membrane has to be treated by cleaning chemicals. The current settings for filtration and cleaning of the membrane are quite conservative and are often based on rules of thumb and pilot plant studies. A more systematic approach to determine optimal settings for membrane filtration came in the 1990s with the work of Van Boxtel et al. [1,2], who used dynamic optimization theory to control fouling in a reverse osmosis installation. Also Perrot [3] applied the dynamic optimization approach to a micro filtration plant processing sugar. In recent studies dynamic optimization of a filtration trajectory of a dead-end ultra filtration plant processing surface water was reported by Blankert et al. [4,5]. Although optimization of filtration and cleaning of membranes over multiple production cycles has been reported in the literature as well [6–8], the aspect of optimal chemical cleaning of a membrane only

received limited attention. In this study we consider the earlier reported and experimentally validated process model by Zondervan et al. [9], describing the fouling state and cleaning agent state as function of time, concentration and cleaning flow, the model is used together with an appropriate performance index (based on the consumption of chemicals and water) and a set of constraints (based on the maximal cleaning flow and concentration) to determine optimal trajectories for the specified control variables (the cleaning flow and cleaning agent concentration).

The optimization objective is to find the optimal profiles for the cleaning flux and cleaning agent concentration as function of time, guaranteeing that a target fouling state is reached within a specified cleaning time, while minimizing the cleaning costs. The problem is schematically represented in Fig. 1.

1.1. The process model

The cleaning model presented in this study is developed in terms of macroscopic component balances. One balance describing the irreversible fouling state and one balance describing the cleaning agent state. It is assumed that the irreversible fouling on the membrane is converted to unspecified decomposition products as a result of exposure to cleaning chemicals. Irreversible fouling is in this context defined as fouling that can not be removed by means of hydraulic cleaning. The decay of

* Corresponding author. Tel.: +31 6 23978639.

E-mail address: zondervan.edwin@gmail.com (E. Zondervan).

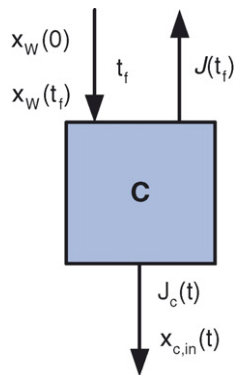


Fig. 1. Schematic representation of the optimization problem. Optimal trajectories for the cleaning flux J_C and the cleaning agent concentration $x_{C,in}$ are calculated, guaranteeing that from an initial fouling state $x_{W,0}$ a target fouling state x_{W,t_f} is reached within a specified cleaning time t_f , while minimizing the cleaning costs.

irreversible fouling is described by:

$$\frac{dx_W}{dt} = -k' J_C (x_W - x_{W,\infty}) + r_W'' \quad (1)$$

where k' is a flushing rate constant, J_C is the dimensionless cleaning flux. $x_{W,\infty}$ is the irreversible fouling state at infinite cleaning time and r_W'' is a first order cleaning rate equation, defined as:

$$r_W'' = -k'' x_C (x_W - x_{W,\infty}) \quad (2)$$

where k'' is a cleaning rate constant which may be temperature dependent and x_C is the cleaning agent state. Note that the ratio k'/k'' defines which aspect of the cleaning is of importance. If $k'/k'' > 1$, the mechanical aspect (flushing) is important, while if $k'/k'' < 1$, the chemical aspect dominates. The cleaning agent state is described by:

$$\frac{dx_C}{dt} = k' J_C (x_{C,in} - x_C) + n_C r_W'' \quad (3)$$

where x_C is the dimensionless cleaning agent concentration.

The following initial conditions hold:

$$x_W(0) = x_{W,0} \quad (4)$$

and

$$x_C(0) = 0 \quad (5)$$

1.2. The performance index

Dynamic optimization of the chemical cleaning phase comprises minimization of a performance index, written in the Lagrange form:

$$\min_{J_C, x_{C,in}} \mathcal{J}(t) = \int_0^{t_f} (w_1 J_C x_{C,in} + w_2 J_C) dt \quad (6)$$

where t_f is the final time and where w_1 and w_2 are the costs for chemicals and permeate. The first term in the performance index represents the costs for the chemicals, the second term represents the costs of permeate usage.

1.3. The constraints

The controls are subject to certain constraints, the cleaning flux can not exceed a specified maximum cleaning flux $J_{C,max}$:

$$0 \leq J_C \leq J_{C,max}; \quad t \in [0, t_f] \quad (7)$$

and the cleaning agent concentration may not exceed a specified maximum cleaning agent concentration, $x_{C,in,max}$:

$$0 \leq x_{C,in} \leq x_{C,in,max}; \quad t \in [0, t_f] \quad (8)$$

At the final time t_f a target fouling status x_{W,t_f} should be reached, which leads to the following equality constraint:

$$x_W(t_f) = x_{W,t_f} \quad (9)$$

1.4. The minimum principle

To solve the dynamic optimization problem, Pontryagin's minimum principle is used. The Hamiltonian can be defined as:

$$\mathcal{H} = \lambda_W \frac{dx_W}{dt} + \lambda_C \frac{dx_C}{dt} + \lambda_J \frac{dJ}{dt} \quad (10)$$

where, λ_W , λ_C and λ_J are the adjointed variables. The conditions for optimality require the derivatives of the Hamiltonian with respect to the controls to be zero:

$$\frac{\partial \mathcal{H}}{\partial J_C} = \frac{\partial \mathcal{H}}{\partial x_{C,in}} = 0 \quad (11)$$

However, the controls appear bilinear and bounded in the Hamiltonian, implying that the optimal values for the controls are zero or maximal (often referred to as 'bang-bang-control' or 'maximum effort control'):

$$J_C(t) = \begin{cases} J_{C,max} & 0 \leq t \leq t^* \\ 0 & t^* \leq t \leq t_f \end{cases} \quad (12)$$

and

$$x_{C,in}(t) = \begin{cases} x_{C,in,max} & 0 \leq t \leq t^* \\ 0 & t^* \leq t \leq t_f \end{cases} \quad (13)$$

The time during which the controls are at their maximum values is called flushing, the time during which the controls are zero is called soaking. The only concern now is to locate the switching point t^* , assuming that both controls have the same switching point. The switching point guaranteeing that the constraint of Eq. (7) is fulfilled depends on the final time. The problem to be solved is how the relationship is between the switching point, the final time and the cleaning effectiveness is, which is defined as:

$$\eta = \frac{x_W(0) - x_W(t_f)}{x_W(0) - x_{W,\infty}} \quad (14)$$

2. Results and discussion

2.1. Simulation

Based on experimental data, the following process model parameter settings are suggested and used: $k' = 1.0$; $k'' = 3.0$; $n_C = 0.01$ and $x_{W,\infty} = 0.05$. The constraints are set to $J_{C,\max} = x_{C,\text{in},\max} = 1$ due to normalization of the problem. The normalized weight factors of the performance index are set to $w_1 = 0.012$ and $w_2 = 0.008$, calculated from the costs of chemicals which are 80 €/m^3 and the costs of permeate which are 0.20 €/m^3 .

In Fig. 2, the fouling state with respect to the controls is represented for different switching points. The dashed horizontal lines in the upper figures represent the requested final fouling state. If the switching point is located at $t^* = 0.5 \text{ min}$ (left figure) the fouling state does not reach the target within 5 min, if the switching point is shifted to $t^* = 1.0 \text{ min}$ the fouling state comes close to its target (middle figure), while for a switching point at $t^* = 1.5 \text{ min}$, the target is reached at around $t = 2.5\text{--}3.0 \text{ min}$ (right figure).

2.2. The relationship between the switching point and the final time

The relationship between the switching point and the final time is best evaluated by means of a numerical algorithm that minimizes the difference between the final fouling conditions and its constraint. First the initial fouling state and the requested

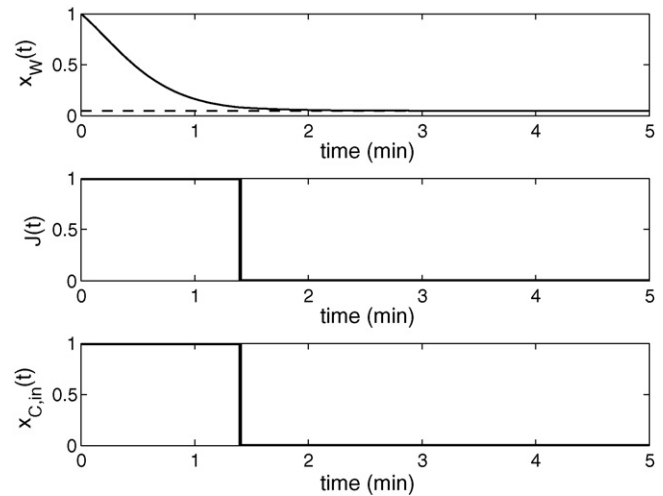


Fig. 3. Typical profile for fouling state and controls for $x_{W,0} = 1.0$ and $x_{W,t_f} = 0.05$.

final fouling state are fixed. Secondly an initial value for the final time and switching point are set. Then, the ODE system of Eqs. (1), (3) and (4) is solved using a MATLAB ODE45 solver, subsequently, the calculated final fouling state is compared to the requested final fouling state. If the final fouling state condition is fulfilled, the final time and its related switching point are stored, and a new final time is set for the next calculation step. If the condition is not satisfied, the time of switching is increased and the ODE solving step and condition evaluation step are repeated. A typical profile for fouling state and controls is shown in Fig. 3,

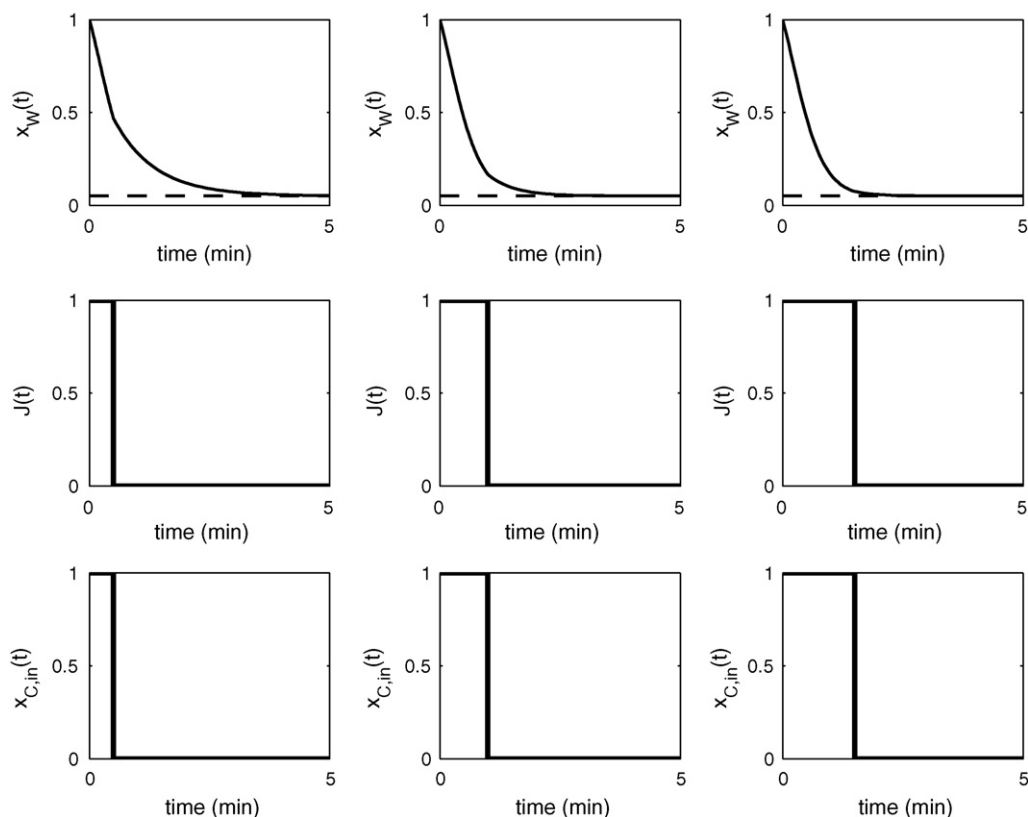


Fig. 2. De fouling state with respect to the controls for different switching points.

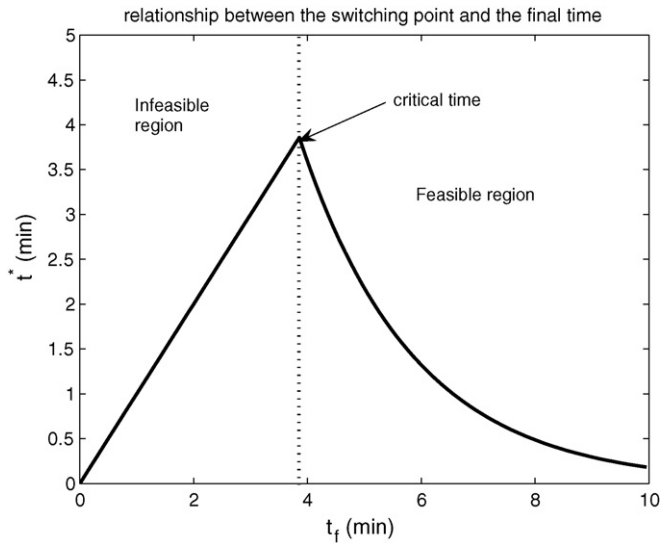


Fig. 4. Relationship between the switching point and the final time for $x_{W,0} = 1.0$ and $x_{W,t_f} = 0.05$.

where the optimal switching point belonging to a final time of 5 min, was found to be 1.3 min, subject to fixed initial and final fouling states. However, if the final time is chosen too short, the requested final fouling state cannot be reached. The routine will consequently calculate for such final time, that the switching point is located at the final time. The time at which the switching time equals the final time, while fulfilling the final fouling constraint is called the critical time. To fulfil the condition set in Eq. (4), the minimum final time equals the critical time. In Fig. 4, the relationship between the final time and the switching point is shown for a fixed initial condition and requested final condition (a fixed cleaning effectiveness), also the critical time is shown in the plot.

2.3. The operating window

The choice of $x_W(t_f)$ (which means the choice of the requested cleaning effectiveness) also influences the location of the switching point, as shown in Figs. 5 and 6.

In the contour plot of Fig. 6, the critical time line ($t_f = t^*$) separates a feasible area from an infeasible area, showing the relationship between t_f and t^* for different values of η . If t_f versus η is plotted, an operating window appears (see Fig. 7), showing which values for η and t_f are allowed. The area between

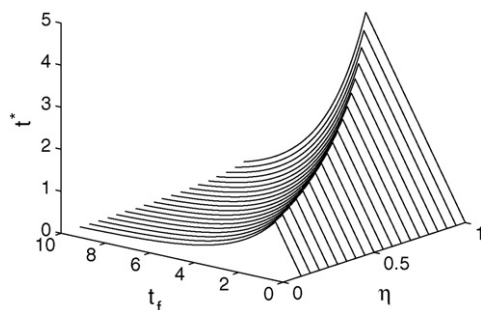


Fig. 5. Surface plot: switching point as function of final time and cleaning effectiveness.

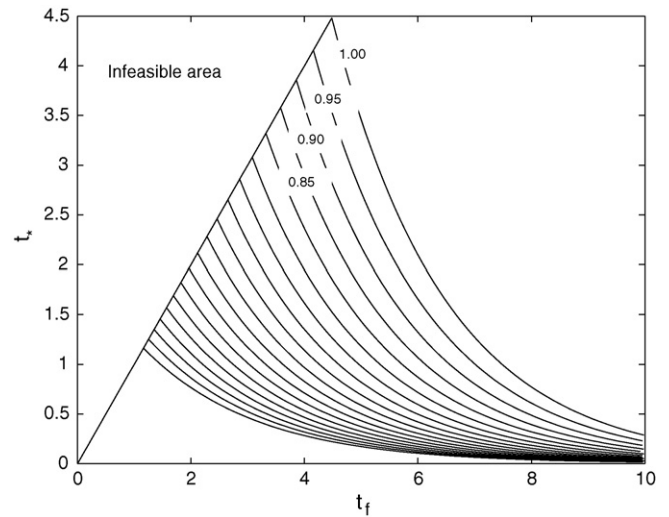


Fig. 6. Contour plot: switching point as function of final time and cleaning effectiveness.

the dashed line and the continuous line mark the feasible region for η and t_f where $t^* < t_f$. In the lower infeasible region, the final fouling condition is not fulfilled and in the upper infeasible region, practical operating conditions cannot be maintained, e.g. the flushing time is too short. If for example $t_f = 10$ min, the optimal switching point would be located at $t^* = 0.3$ min, which means a flushing time of 0.3 min. This time is too short for the pumps to be able to fill the membrane module.

2.4. Evaluation of the cleaning costs

From the performance index of Eq. (4) and the optimal profiles for the controls of Eqs. (10) and (11) it can be seen that:

$$\mathcal{J}(t_f) = \int_0^{t^*} (w_1 J_{C,\max} x_{C,\text{in},\max} + w_2 J_{C,\max}) dt + \int_{t^*}^{t_f} (w_1 \cdot 0 \cdot 0 + w_2 \cdot 0) dt \quad (15)$$

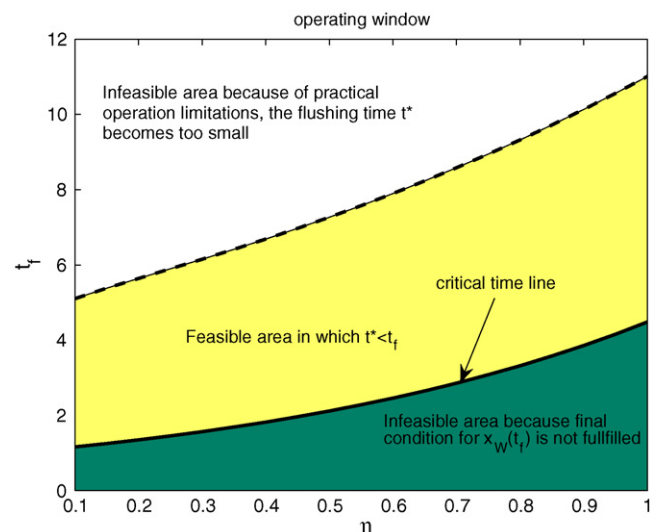


Fig. 7. The operating window.

Because the maximal controls do not change as a function of time, Eq. (15) can be simplified to:

$$\mathcal{J}(t_f) = \alpha \cdot t^* \quad (16)$$

with

$$\alpha = w_1 J_{C, \max} x_{C, \text{in}, \max} + w_2 J_{C, \max} \quad (17)$$

The costs are linearly dependent on the switching point (the quantity of used chemicals). Minimization of the performance index comprises minimization of the switching point, i.e. the switching time should be at its minimum allowable value, while honoring the constraints.

2.5. Comparison to conventional cleaning

A conventional cleaning is on average executed once every 12 h. Chemicals are normally flushed through the module at maximum flux during one minute, and are subsequently left to soak for 30 min. Operational costs of a functioning UF installation are around 0.20 € / m³ produced water. Chemical cleaning costs take up to 5

From Fig. 4 two optimal cleaning procedures are derived, in the first case: $t_f = 3.75$ min with $t^* = 3.75$ min, and in the second case: $t_f = 8.00$ min with $t^* = 0.50$ min. From the first case it follows directly that a major reduction in cleaning time can be made in comparison to a conventional cleaning procedure. From the second case it follows that also a significant reduction in cleaning agent consumption may be realized if a longer cleaning time can be allowed.

3. Conclusions

Dynamic optimization results in a maximum effort control problem, where the optimization problem can be transformed in finding the optimal location of the switching point. A relationship between the switching time, the final time and the cleaning effectiveness was found by means of simulation using an experimentally verified cleaning model. Consequently, an operating window could be formulated. The performance index showed that the costs are minimal if the switching time is chosen as small as possible. From the calculated optimal control strategy it follows that cleaning time can be significantly reduced, compared to conventional cleaning.

Nomenclature

\mathcal{H}	Hamiltonian
\mathcal{J}	performance index (€)
$J_C(t)$	cleaning flow
$J_{C, \max}$	maximum cleaning flow

k'	flushing rate constant (min ⁻¹)
k''	cleaning rate constant (min ⁻¹)
n_C	pseudo stoichiometric constant
t	time (min)
t_f	final cleaning time (min)
t^*	switching point (min)
w_1	cleaning agent costs (€/min)
w_2	permeate costs (€/min)
$x_C(t)$	cleaning agent state
$x_{C, \text{in}}(t)$	cleaning agent concentration at inlet
$x_{C, \text{in}, \max}$	maximum cleaning agent concentration
$x_W(t)$	irreversible fouling state
$x_{W, \infty}$	irreversible fouling state at infinite cleaning

Greek letters

η	cleaning effectiveness
λ_C	adjointed variable with respect to the cleaning state (min)
$\lambda_{\mathcal{J}}$	adjointed variable with respect to the performance index (min/€)
λ_W	adjointed variable with respect to the fouling state (min)

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